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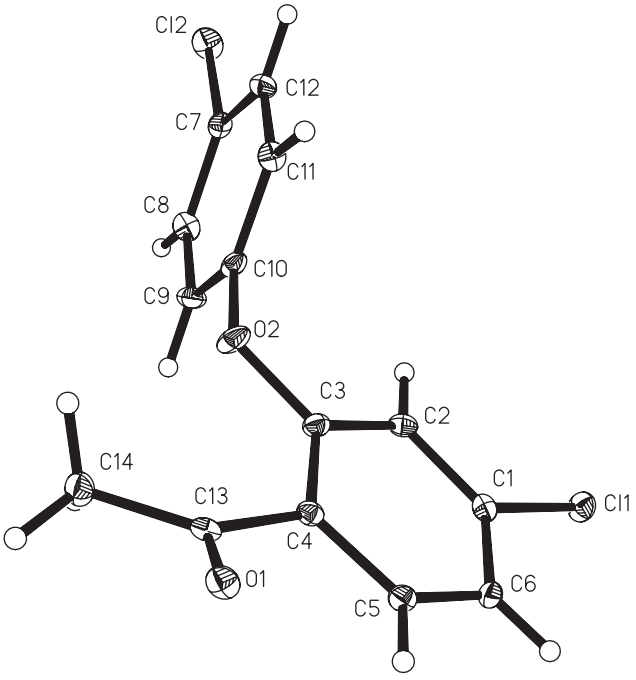
The crystal structure of 1-(2-(4-chlorophenoxy)-4-chlorophenyl)ethanone, $C_{14}H_{10}Cl_2O_2$



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Abstract

$C_{14}H_{10}Cl_2O_2$, monoclinic, $P2_1/c$ (no. 14), $a = 13.448(7)$ Å, $b = 7.6635(5)$ Å, $c = 13.638(6)$ Å, $\beta = 117.14(6)°$, $V = 1250.7(9)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0318$, $wR_{ref}(F^2) = 0.0738$, $T = 104.8$ K.

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The crystal structure is shown in the figure. Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	Colorless, block, size 0.07×0.40×0.40 mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ:	5.08 cm^{-1}
Diffractometer, scan mode:	Xcalibur, Eos, Gemini, ω scans
$2\theta_{max}$:	51.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6320, 2454
$N(param)_{refined}$:	164
Programs:	CrysAlis [6], SHELX [7], OLEX2 [8]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	Site	x	y	z	U_{iso}
H(5)	4*e*	0.4812	0.0601	0.6645	0.019
H(12)	4*e*	−0.1413	−0.1099	0.1176	0.023
H(6)	4*e*	0.4893	0.2858	0.5557	0.020
H(11)	4*e*	−0.0101	−0.0807	0.3015	0.023
H(2)	4*e*	0.2265	0.0774	0.2944	0.021
H(14A)	4*e*	0.3678	−0.4818	0.6363	0.034
H(14B)	4*e*	0.3425	−0.4178	0.5181	0.034
H(14C)	4*e*	0.2482	−0.4138	0.5554	0.034
H(9)	4*e*	0.2224	−0.3059	0.2358	0.024
H(8)	4*e*	0.0925	−0.3315	0.0514	0.025

Source of material

The title compound was prepared by the method described in CN. Pat.No. 101434528A [1]. It was recrystallized from acetone at room temperature to give colorless crystals.

Experimental details

H atoms were positioned geometrically with C—H = 0.93 Å and 0.96 Å for aromatic and methyl, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2$ (or 1.5 for methyl group) times $U_{eq}(C)$.

Discussion

1-(4-(4-chlorophenoxy)-2-chlorophenyl)ethanone is an important intermediate used for the synthesis of agrochemical difenoconazole [2, 3], while 1-(2-(4-chlorophenoxy)-4-chlorophenyl)ethanone is its isomers. According the literature [4, 5], the two compound can't been differentiate. In

Table 3: Atomic displacement parameters (Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl(1)	4*e*	0.36616(4)	0.36565(6)	0.33156(3)	0.0247(2)	0.0192(2)	0.0195(2)	−0.0027(2)	0.0083(2)	0.0041(2)
Cl(2)	4*e*	−0.13584(4)	−0.25297(6)	−0.06849(4)	0.0286(3)	0.0291(3)	0.0138(2)	0.0032(2)	0.0002(2)	−0.0032(2)
O(1)	4*e*	0.3985(1)	−0.1877(2)	0.72094(9)	0.0219(7)	0.0216(6)	0.0127(6)	0.0025(6)	0.0054(5)	0.0005(5)
O(2)	4*e*	0.1919(1)	−0.1878(2)	0.39716(9)	0.0178(7)	0.0271(7)	0.0129(6)	−0.0094(6)	−0.0010(5)	0.0037(5)
C(1)	4*e*	0.3597(1)	0.1983(2)	0.4151(1)	0.0190(9)	0.0147(8)	0.0186(9)	0.0027(7)	0.0105(8)	0.0023(7)
C(5)	4*e*	0.4311(1)	0.0622(2)	0.5899(1)	0.0160(9)	0.0180(9)	0.0124(8)	0.0014(7)	0.0045(7)	−0.0028(7)
C(12)	4*e*	−0.0685(2)	−0.1488(2)	0.1415(1)	0.0150(9)	0.0193(9)	0.0188(9)	0.0021(7)	0.0048(7)	0.0009(7)
C(6)	4*e*	0.4362(2)	0.1978(2)	0.5257(1)	0.0164(9)	0.0141(8)	0.0191(9)	−0.0011(7)	0.0069(7)	−0.0039(7)
C(13)	4*e*	0.3609(1)	−0.2173(2)	0.6227(1)	0.0111(8)	0.0199(9)	0.0144(9)	0.0032(7)	0.0049(7)	0.0011(7)
C(11)	4*e*	0.0097(2)	−0.1321(2)	0.2511(1)	0.022(1)	0.0193(9)	0.0164(9)	0.0006(8)	0.0086(8)	−0.0008(7)
C(2)	4*e*	0.2781(1)	0.0721(2)	0.3685(1)	0.0133(9)	0.0216(9)	0.0131(8)	0.0016(7)	0.0031(7)	0.0018(7)
C(14)	4*e*	0.3268(2)	−0.3991(2)	0.5792(2)	0.026(1)	0.0185(9)	0.0169(9)	−0.0005(8)	0.0046(8)	0.0015(7)
C(4)	4*e*	0.3529(1)	−0.0715(2)	0.5463(1)	0.0138(8)	0.0161(8)	0.0134(8)	0.0022(7)	0.0057(7)	−0.0010(7)
C(10)	4*e*	0.1171(1)	−0.1923(2)	0.2847(1)	0.0158(9)	0.0172(9)	0.0125(8)	−0.0054(7)	0.0009(7)	0.0025(7)
C(3)	4*e*	0.2747(1)	−0.0626(2)	0.4350(1)	0.0130(8)	0.0180(9)	0.0150(9)	−0.0012(7)	0.0045(7)	−0.0022(7)
C(7)	4*e*	−0.0364(2)	−0.2244(2)	0.0681(1)	0.0185(9)	0.0164(9)	0.0119(8)	−0.0023(7)	0.0021(7)	−0.0004(7)
C(9)	4*e*	0.1495(2)	−0.2668(2)	0.2116(2)	0.0123(9)	0.024(1)	0.023(1)	0.0021(8)	0.0069(7)	0.0055(7)
C(8)	4*e*	0.0720(2)	−0.2825(2)	0.1020(2)	0.025(1)	0.021(1)	0.0191(9)	0.0026(8)	0.0120(8)	0.0012(7)

order to distinguish the two compound, in this paper, the title compound was separated and its structure was characterized. As shown in the figure there are two diffrently substituated phenyl moieties in the molecular structure. The dihedral angle between two rings is 83.3°.

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References

1. Wang, L.: Difenoconazole azole preparation process. CN200710177383.X, 2007.
2. Sekimata, K.; Han, S. Y.; Yoneyama, K.; Takeuchi, Y.; Yoshida, S.; Asami, T.: A specific and potent inhibitor of brassinosteroid biosynthesis possessing a dioxolane ring. J. Agric. Food Chem. **50** (2002) 3486–3490.
3. Rueegg, J.; Siegfried, W.: Residues of difenoconazole and penconazole on apple leaves and grass and soil in an apple orchard in north-eastern Switzerland. Crop Prot. **15** (1996) 27–31.
4. Lan, Z.: Catalytic synthesis of 4-(4-chlorophenoxy)-2-chlorophenyl ethanone and microwave promotion in the reaction. Chinese J. Appl. Chem. **19** (2002) 346–350.
5. Li, H.; Liao, F.; Wang, P.; et al.: Preparation of fungicide difenoconazole. Trans. Beijing Institute Technol. **26** (2006) 365–368.
6. Agilent Technologies: CrysAlis PRO Software System, Version 1.171.35.15, Agilent Technologies UK Ltd, Oxford, UK, 2011.
7. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112–122.
8. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H.: OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Cryst. **42** (2009) 339–341.